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G. F. Dresselhaus

Ferro- and Antiferromagnetism in a Cubic Cluster of Spins

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FERRO- AND ANTIFERROMAGNETISM IN A CUBIC CLUSTER OF SPINS

G. F. DRESSELHAUS

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ABSTRACT

The Heisenberg exchange Hamiltonian has been solved exactly for a cubic array of eight spins (each with spin 1/2). Both energy eigenvalues and thermodynamic functions have been calculated. A Curie and a Néel temperature can be defined and their values determined as a function of the strength of first, second and third neighbor interactions. For some values of the exchange constants, "spiral" antiferromagnetic states exist.

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FERRO- AND ANTIFERROMAGNETISM IN A CUBIC CLUSTER OF SPINS

I. INTRODUCTION

The exact three-dimensional solution of the Heisenberg model for ferromagnetism is not tractable for an infinite lattice. There are various approximate solutions, some of which involve the exact solution for some small cluster of spins.[1,2] In addition, a number of solutions exist in the literature for a small number of spins in various configurations.[3] This report gives the exact solution to the Heisenberg Hamiltonian for eight spins, each with spin 1/2, located on the corners of a cube. Both the eigenvalues and the thermodynamic functions have been calculated.

This simple cluster shows many of the features of an infinite magnetic material. In particular, a ferromagnetic Curie temperature T_C and an antiferromagnetic Néel temperature T_N can be defined, and their values computed as a function of the strength of second and third neighbor interactions. It is shown that, for some values of the interactions, "spiral" antiferromagnetic states exist.[4] It is also shown that there are regions in which, as the temperature is lowered, ferromagnetic ordering begins, but at still lower temperatures, the system drops into the antiferromagnetic singlet state.

The approximate solution to the infinite simple cubic lattice, using the results contained herein, will be published in a subsequent report.

II. CALCULATION

The Heisenberg Hamiltonian is written

$$\mathcal{H} = -2J[\epsilon + x\mu + y\nu] \tag{1}$$

in which J is the exchange constant, x and y are proportional to the strength of next nearest and third nearest neighbor interactions, and

$$\begin{aligned}
\epsilon &= \vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_3 \cdot \vec{S}_4 + \vec{S}_4 \cdot \vec{S}_1 + \vec{S}_5 \cdot \vec{S}_6 + \vec{S}_6 \cdot \vec{S}_7 + \vec{S}_7 \cdot \vec{S}_8 + \vec{S}_8 \cdot \vec{S}_5 \\
&\quad + \vec{S}_1 \cdot \vec{S}_5 + \vec{S}_2 \cdot \vec{S}_6 + \vec{S}_3 \cdot \vec{S}_7 + \vec{S}_4 \cdot \vec{S}_8 \quad , \\
\mu &= \vec{S}_1 \cdot \vec{S}_3 + \vec{S}_2 \cdot \vec{S}_4 + \vec{S}_5 \cdot \vec{S}_7 + \vec{S}_6 \cdot \vec{S}_8 + \vec{S}_1 \cdot \vec{S}_6 + \vec{S}_2 \cdot \vec{S}_7 + \vec{S}_3 \cdot \vec{S}_8 + \vec{S}_4 \cdot \vec{S}_5 \\
&\quad + \vec{S}_1 \cdot \vec{S}_8 + \vec{S}_2 \cdot \vec{S}_5 + \vec{S}_3 \cdot \vec{S}_6 + \vec{S}_4 \cdot \vec{S}_7 \quad , \\
\nu &= \vec{S}_1 \cdot \vec{S}_7 + \vec{S}_2 \cdot \vec{S}_8 + \vec{S}_3 \cdot \vec{S}_5 + \vec{S}_4 \cdot \vec{S}_6 \quad .
\end{aligned} \tag{2}$$

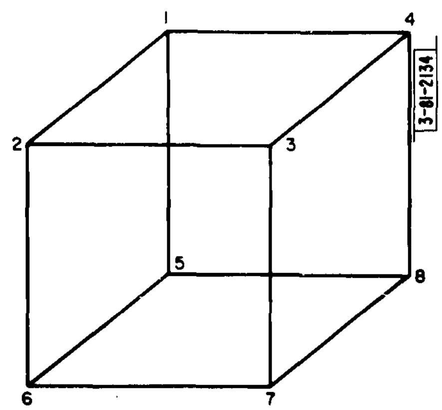

Fig. 1. Cube showing the numbering of the spins.

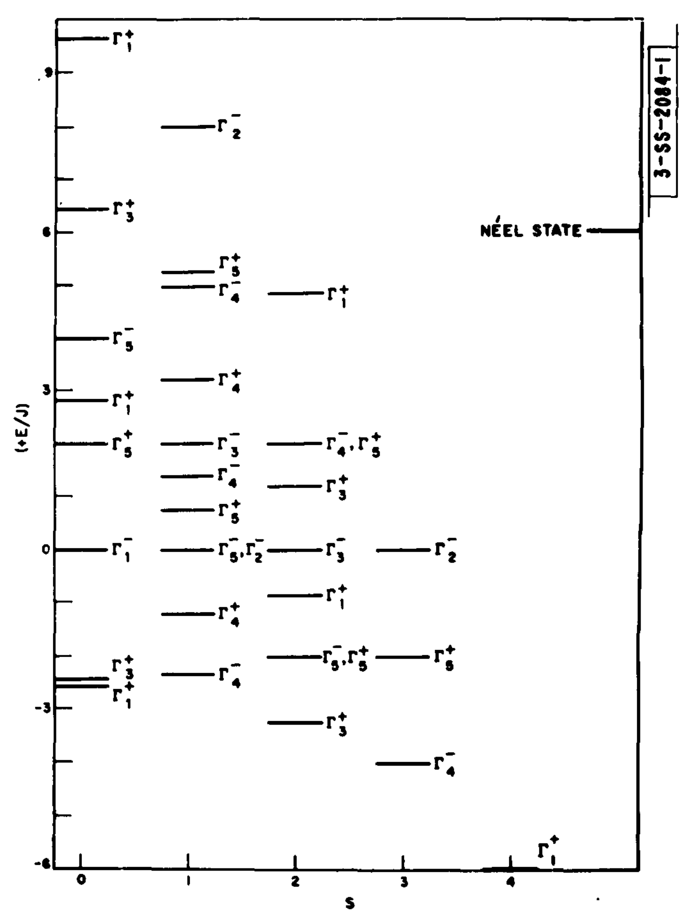

Fig. 2. Energy spectrum assuming only nearest neighbor interactions, x = y = 0. The spectrum is arranged according to the value of the total spin. The Néel state energy is indicated even though it is not a proper eigenstate of the system.

The spin operator for the i^{th} site $\vec{S}_i$ follows the numbering of the sites shown in Fig. 1.

The eigenfunctions of Eq. (1) can be classified according to the total spin S, the z-component of the total spin M_S, and the irreducible representation of the cubic group. Table I lists the symmetry types and energy eigenvalues for the cubic cluster.[5] Appendix A tabulates the wave functions. Appendix B gives the matrix elements of $\epsilon + x\mu + y\nu$ for the wave functions of Appendix A. The notation for the representations is such that a vector transforms as Γ_4^-. The spectrum for $x = y = 0$ is shown in Fig. 2.

For a given value of the total spin S, the center of gravity of the energy levels E_{CG} is given by the sum rule

$$E_{CG} = -2\left[\sum_{i<j} J_{ij}\right][S(S+1) - (3/4)\,N]/[N(N-1)] \tag{3}$$

in which N is the number of spins (each with spin 1/2) and J_{ij} is the exchange constant between sites i and j. Equation (3) represents a convenient check of the calculated energy eigenvalues. The Heisenberg approximation for ferromagnetism[6] corresponds to calculating the partition function, using Eq. (3) for the energy eigenvalues.

The partition function for the cubic cluster is calculated by using the eigenfunctions listed in Table I. From the partition function, the susceptibility and heat capacity for the system are calculated. The susceptibility χ given by the Curie law is written as

$$\chi = NS(S+1)\,\frac{g^2\mu_B^2}{3kT} \tag{4}$$

in which N is the number of spins, S is the spin quantum number $g = 2$ and μ_B is the Bohr magneton. The cubic cluster obeys the Curie law with suitable identification of N and S. For high temperatures, $2J/kT \ll 1$, the necessary interpretation of N and S is

$$NS(S+1) = 6 \quad ,$$

and at low temperatures, $2J/kT \gg 1$, the interpretation is changed to $N = 1$ with

$$NS(S+1) = 20 \qquad J > 0$$

and

$$NS(S+1) = 0 \qquad J < 0 \quad .$$

A plot of the susceptibility vs $1/T$ for $x = y = 0$ is shown in Fig. 3 for both the ferromagnetic and antiferromagnetic states. For convenience, the plot is presented in dimensionless form in terms of $\alpha\chi$ vs $2J/kT$, with $\alpha = 6J/g^2\mu_B^2$. For the ferromagnetic case ($J > 0$) the slope of the curve in Fig. 3(a) has the two asymptotic values indicated by the dashed lines. The ferromagnetic Curie temperature T_C is defined as the position of maximum slope of the χ vs $1/T$ curve. The antiferromagnetic Néel temperature T_N is defined as the position of the maximum in the susceptibility curve. With these definitions, the Curie and Néel temperatures have been determined as a function of x and y. These results are shown in Fig. 4.

The heat capacity is shown for the same parameters in Fig. 5. The positions of T_C and T_N, as determined from the susceptibility, are also indicated. The maximum of the heat capacity curves differs somewhat from T_C and T_N, as determined from the susceptibility.

TABLE 1

SPIN, SYMMETRY TYPE AND ENERGY EIGENVALUES FOR THE CUBIC CLUSTER OF EIGHT SPINS

Spin	Representation	Eigenvalue ($\lambda = E/(-2J)$)
4	Γ_1^+	$\lambda = 3 + 3x + y$
3	Γ_4^-	$\lambda = 2 + x$
	Γ_5^+	$\lambda = 1 + x + y$
	Γ_2^-	$\lambda = 3x$
2	Γ_3^+	$\lambda = \frac{1}{2}(1-x) \pm \frac{1}{2}[(1-x)^2 + 4(1-y)^2]^{1/2}$
	Γ_3^+	
	Γ_5^+	$\lambda = \pm[(1-x)^2 + (1-y)^2 - (1-x)(1-y)]^{1/2}$
	Γ_5^+	
	Γ_1^+	$\lambda = -(1-x) \pm [4(1-x)^2 + (1-y)^2 - 3(1-x)(1-y)]^{1/2}$
	Γ_1^+	
	Γ_5^-	$\lambda = 1 - x$
	Γ_4^-	$\lambda = -1 + x$
	Γ_3^-	$\lambda = 0$

TABLE I (Continued)

SPIN, SYMMETRY TYPE AND ENERGY EIGENVALUES
FOR THE CUBIC CLUSTER OF EIGHT SPINS

Spin	Representation	Eigenvalue ($\lambda = E/(-2J)$)
1	Γ_4^-	$\lambda^3 + 2\lambda^2(1 + x + y) + \lambda(-2 + 7x + 5y + 3xy - x^2) + (-2 + 2y + 4x^2 + 6xy - 2x^3) = 0$
	Γ_4^-	
	Γ_4^-	
	Γ_4^+	$\lambda = -\frac{1}{2}(1 + 3x) \pm \frac{1}{2}[5 - 2x + x^2 + 4y^2 - 8y]^{1/2}$
	Γ_4^+	
	Γ_2^-	$\lambda = -2 + x - y \pm [4 - 7x - y + 4x^2 + y^2 - xy]^{1/2}$
	Γ_2^-	
	Γ_5^+	$\lambda = -\frac{1}{2}(3 + x) \pm \frac{1}{2}[5 - 10x + 9x^2 - 8xy + 4y^2]^{1/2}$
	Γ_5^+	
	Γ_5^-	$\lambda = -2x$
	Γ_3^-	$\lambda = -1 - x$
0	Γ_1^+	$\lambda^3 + \lambda^2(5 + x + 3y) + \lambda(-1 + 18x + 14y - 9x^2 + 6xy - y^2) + 3(-9 + 3x + 5y + 3x^2 + 6xy - y^2 - 3x^3 - 3x^2y + 3xy^2 - y^3) = 0$
	Γ_1^+	
	Γ_1^+	
	Γ_3^+	$\lambda = -(1 + 2x) \pm [2 - 2x + x^2 - 2y + y^2]^{1/2}$
	Γ_3^+	
	Γ_1^-	$\lambda = -3x$
	Γ_5^+	$\lambda = -(1 + x + y)$
	Γ_5^-	$\lambda = -2 - x$

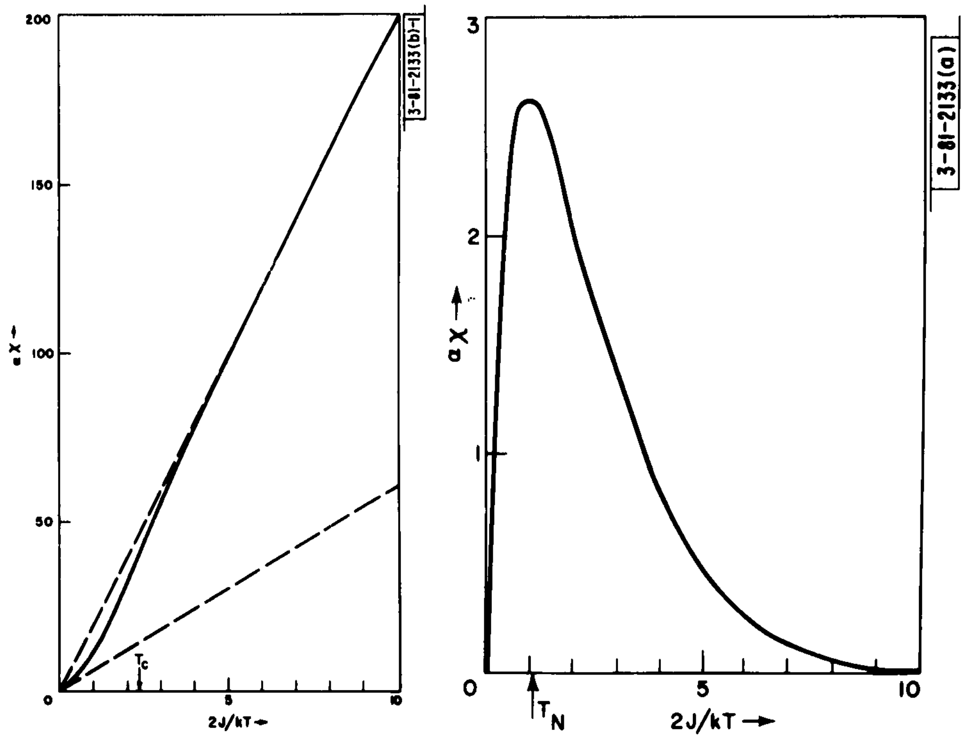

Fig. 3. Susceptibility vs 2J/kT for (a) $J > 0$ and (b) $J < 0$ and $x = y = 0$. The Curie and Néel temperatures are indicated. See text for constant of proportionality, a.

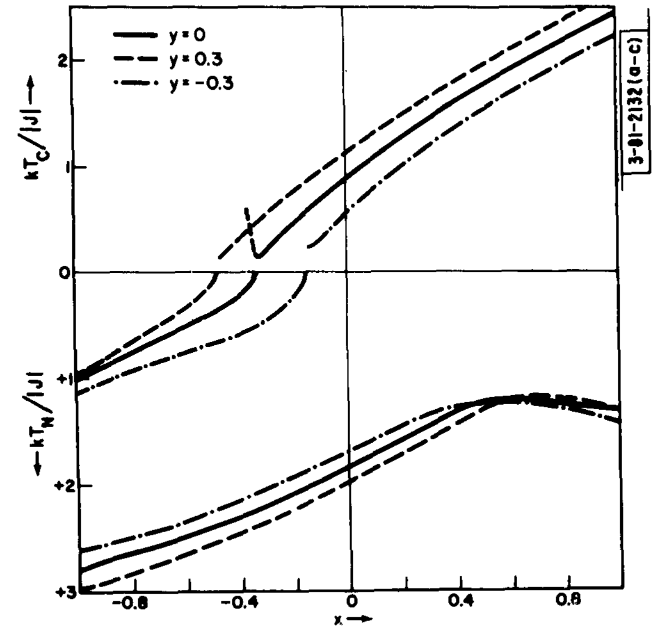

Fig. 4. T_C and T_N vs x with y as a parameter. The upper curves refer to $J > 0$ and the lower curves to $J < 0$.

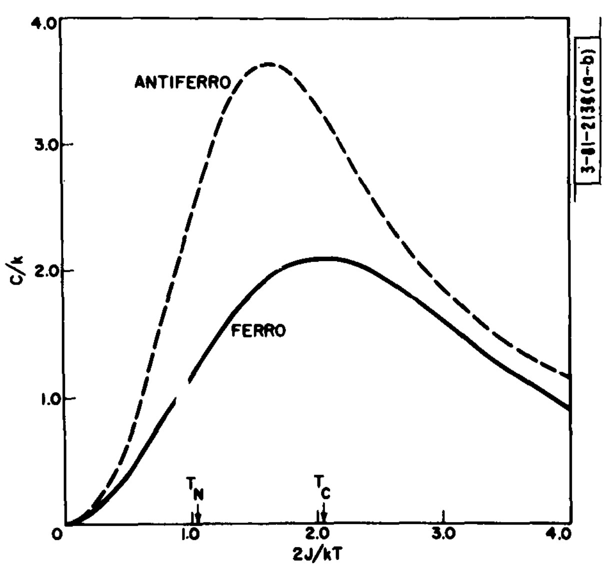

Fig. 5. Heat capacity vs 2J/kT for x = y = 0. T_C and T_N as determined from the susceptibility are indicated.

III. DISCUSSION

The calculation of the magnetic properties for an 8-spin cub
esting features. The antiferromagnetic state gives a good appr
netic state of the infinite solid. The susceptibility and heat cap
high-temperature limits as the infinite lattice. For $x = y = 0$, t
determined from the susceptibility of the 8-spin cluster is given
with the Bethe, Peierls, Weiss value of 2.01 (see Ref. 1). The fe
hand, is not well represented by the small cluster. The heat ca
high-temperature limits, but the susceptibility has the correct l
temperature case (paramagnetic region). In addition, the Curie
given by $kT_C/J = 0.90$ compared with the Bethe, Peierls, Weiss

In order to investigate the number of spins required to repr
of an infinite solid, the Heisenberg approximation (i.e., assume
carried out for clusters of 8, 64 and 216 spins. The results for
Fig. 6. The Curie temperature for these clusters was found fror
the results are shown in Table II. A rather slow convergence is
netic case. To put it another way, 216 spins are too few to repr
lattice. The results for the cluster show that fewer spins are ne
magnetic state than the ferromagnetic state. Comparison with tl
not useful for the antiferromagnetic case. The Heisenberg appro
antiferromagnetic state which get worse as N increases; that is

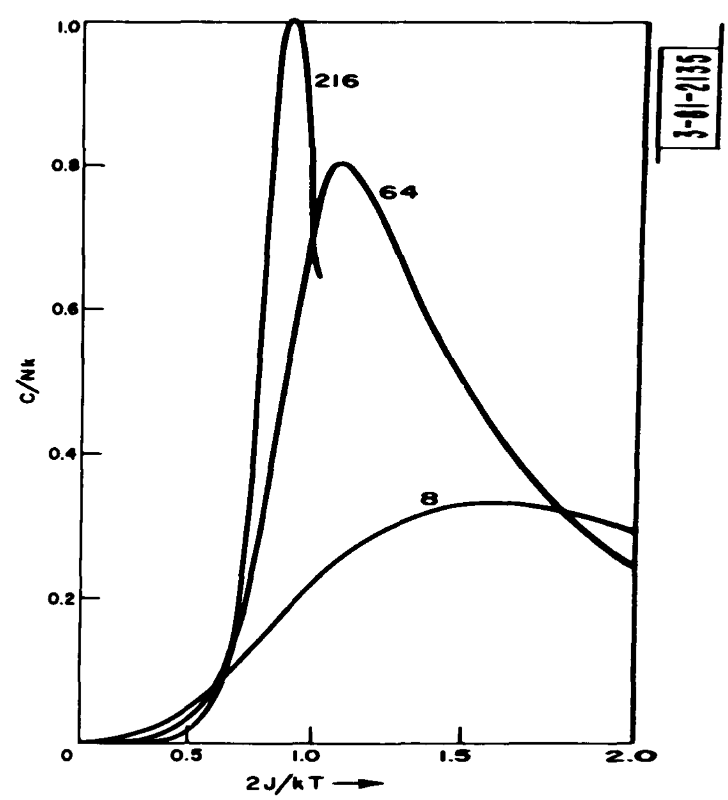

Fig. 6. Heat capacity for
Heisenberg approximation
216 spins.

TABLE II

VALUES OF T_C CALCULATED IN THE HEISENBERG APPROXIMATION FOR CUBIC CLUSTERS OF VARIOUS NUMBERS OF SPINS

N	kT_C/J
8	1.3
64	1.8
216	2.2
.	.
.	.
.	.
∞	3.0

Another interesting feature of the 8-spin cubic cluster is the existence of an antiferromagnetic state for $J > 0$. For example, for $y = 0$ and $x < -1/3$, an antiferromagnetic state exists with $J > 0$, which corresponds to a "classical" spiral state;[4] that is, nearest neighbors are mostly parallel to take advantage of positive J and next nearest neighbors are mostly antiparallel. An examination of the susceptibility curve in the region $y = 0$ and $x \lesssim -1/3$ shows that the system begins to order ferromagnetically because of the greater weighting factor for the $S = 4$ state, but at low temperatures, the system becomes antiferromagnetic because an $S = 0$, Γ_1^+ state is lower in energy.[7] The condition on x and y for the accidental degeneracy of the $S = 4$, Γ_1^+ state and an $S = 0$, Γ_1^+ state is given by

$$3(1 + 4x_o + 3x_o^2) + 7y_o + 12x_oy_o + 2y_o^2 + 3x_o^2y_o + 2x_oy_o^2 = 0 \quad . \qquad (5)$$

In Fig. 4, the dashed branch of the $y = 0$ curve indicates this possibility of a "high" temperature ferromagnetic state. The $y = \pm 0.3$ calculations also allow this possibility but, for simplicity, these branches are not plotted in Fig. 4.

It is also possible to select values of the parameters x and y so that an $S = 0$, Γ_3^+ state is the lowest antiferromagnetic state of the system for $J < 0$. The classical analog to this situation is discussed in Ref. 4.

ACKNOWLEDGMENT

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2. J.S. Smart, J. Phys. Chem. Solids 20, 41 (1961).
3. R. Orbach, Phys. Rev. 115, 1181 (1959); L.F. Mattheiss, Phys. Rev. 123, 1209 (1961).
4. T.A. Kaplan, Phys. Rev. 116, 888 (1959); J. Villain, J. Phys. Chem. Solids 11, 303 (1959); A. Yoshimori, J. Phys. Soc. Japan 14, 807 (1959).
5. The notation for the irreducible representations is $\Gamma_1^+ \rightarrow 1$; $\Gamma_2^- \rightarrow xyz$; $\Gamma_3^+ \rightarrow x^2 + \omega y^2 + \omega^2 z^2,\ x^2 + \omega^2 y^2 + \omega z^2$; $\Gamma_4^- \rightarrow x, y, z$; and $\Gamma_5^+ \rightarrow yz, xz, xy$.
6. J.H. VanVleck, Electric and Magnetic Susceptibilities (Oxford University Press, London, England, 1932) p. 322.
7. This effect has many of the same features as that used by H. Sato and A. Arrott, Phys. Rev. 114, 1427 (1959), to explain the magnetic behavior of some Fe-Al alloys which are ferromagnetic at high temperatures but antiferromagnetic at low temperatures.

APPENDIX A
EIGENFUNCTIONS OF THE 8-SPIN PROBLEM

The notation is as follows:

spin configuration (137) ≡ $\beta(1)\ \alpha(2)\ \beta(3)\ \alpha(4)\ \alpha(5)\ \alpha(6)\ \beta(7)\ \alpha(8)$

in which $\alpha(i) \rightarrow$ spin "i" up and $\beta(i) \rightarrow$ spin "i" down. Only the maximum M_S state is listed, since the lower M_S states can be obtained by application of a lowering operator. For the representations $\Gamma_3^{\pm}$, only one eigenfunction is given; the other can be obtained by taking the complex conjugate of the given function. For $\Gamma_4^{\pm}$ and $\Gamma_5^{\pm}$, only one function is given; the other two can be obtained by performing the appropriate symmetry operations. When the same representation occurs several times, a lower case Greek letter is used to distinguish the representation. An "i" is used to label the state in the case of a multidimensional representation.

The states are eigenstates of S^2 and S_z but not necessarily of $\mathcal{H}$. The wave function is a sum of the spin configurations. The coefficient of each spin configuration is given in Table A-I. The absolute value of the square of the wave function is the last entry in the table.

TABLE A-I
NUMERICAL COEFFICIENTS OF THE VARIOUS SPIN CONFIGURATIONS

S = 3			
Spin Configuration	Γ_2^-	$\Gamma_4^- i$	$\Gamma_5^+ i$
(1)	+	–	–
(2)	–	+	–
(3)	+	+	+
(4)	–	–	+
(5)	–	–	+
(6)	+	+	+
(7)	–	+	–
(8)	+	–	–
$\lvert\Gamma_i\rvert^2$	8	8	8

TABLE A-I (Continued)

NUMERICAL COEFFICIENTS
OF THE VARIOUS SPIN CONFIGURATIONS

S = 2

Spin Configuration	$\Gamma_1^+\alpha$	$\Gamma_1^+\beta$	$\Gamma_3^+\alpha, i$	$\Gamma_3^+\beta, i$	Γ_3^-i	Γ_4^-i	$\Gamma_5^+\alpha, i$	$\Gamma_5^+\beta, i$	Γ_5^-i
(12)	+	+	1			+			+
(23)	+	+	ω			+			−
(34)	+	+	1			+			+
(14)	+	+	ω			+			−
(56)	+	+	1			−			−
(67)	+	+	ω			−			+
(78)	+	+	1			−			−
(58)	+	+	ω			−			+
(15)	+	+	ω^2				+	+	
(26)	+	+	ω^2				−	−	
(37)	+	+	ω^2				+	+	
(48)	+	+	ω^2				−	−	
(17)		−6						−2	
(28)		−6						+2	
(35)		−6						−2	
(46)		−6						+2	

TABLE A-I (Continued)

NUMERICAL COEFFICIENTS
OF THE VARIOUS SPIN CONFIGURATIONS

S = 2

Spin Configuration	$\Gamma_1^+\alpha$	$\Gamma_1^+\beta$	$\Gamma_3^+\alpha, i$	$\Gamma_3^+\beta, i$	$\Gamma_3^- i$	$\Gamma_4^- i$	$\Gamma_5^+\alpha, i$	$\Gamma_5^+\beta, i$	$\Gamma_5^- i$
(13)	–	+		1	1	–2	–	+	
(24)	–	+		1	–1	–2	+	–	
(57)	–	+		1	–1	2	–	+	
(68)	–	+		1	1	2	+	–	
(27)	–	+		ω^2	$-\omega^2$				
(36)	–	+		ω^2	ω^2				
(18)	–	+		ω^2	ω^2				
(45)	–	+		ω^2	$-\omega^2$				
(38)	–	+		ω	ω				
(47)	–	+		ω	$-\omega$				
(25)	–	+		ω	$-\omega$				
(16)	–	+		ω	ω				
$\lvert\Gamma_i\rvert^2$	24	168	12	12	12	24	8	24	24

where $\omega^3 = 1$.

TABLE A-I (Continued)

NUMERICAL COEFFICIENTS
OF THE VARIOUS SPIN CONFIGURATIONS

S = 1

Spin Configuration	$\Gamma_2^-\alpha$	$\Gamma_2^-\beta$	$\Gamma_3^- i$	$\Gamma_4^+\alpha, i$	$\Gamma_4^+\beta, i$	$\Gamma_4^-\alpha, i$	$\Gamma_4^-\beta, i$	$\Gamma_4^-\gamma, i$	$\Gamma_5^+\alpha, i$	$\Gamma_5^+\beta, i$	$\Gamma_5^- i$
(123)	+	–	1			–	–1/2	–1/3	–	–	
(134)	+	–	1			–	–1/2	–1/3	–	–	
(568)	+	–	1			+	1/2	1/3	+	+	
(678)	+	–	1			+	1/2	1/3	+	+	
(236)	+	–	$-\omega$	+			+	1/6		+	+
(126)	+	–	$+\omega^2$	–			+	1/6		+	–
(367)	+	–	$-\omega$	–			–	–1/6		–	–
(348)	+	–	ω^2	–			+	1/6		+	–
(378)	+	–	ω^2	+			–	–1/6		–	+
(158)	+	–	$-\omega$	–			–	–1/6		–	–
(156)	+	–	ω^2	+			–	–1/6		–	+
(148)	+	–	$-\omega$	+			+	1/6		+	+
(234)	–	+	–1			–	–1/2	–1/3	+	+	
(124)	–	+	–1			–	–1/2	–1/3	+	+	
(267)	–	+	ω	+			–	–1/6		+	–
(145)	–	+	ω	–			+	1/6		–	+
(256)	–	+	$-\omega^2$	–			–	–1/6		+	+
(347)	–	+	$-\omega^2$	+			+	1/6		–	–
(578)	–	+	–1			+	1/2	1/3	–	–	
(567)	–	+	–1			+	1/2	1/3	–	–	
(125)	–	+	$-\omega^2$	+			+	1/6		–	–
(478)	–	+	$-\omega^2$	–			–	–1/6		+	+
(237)	–	+	ω	–			+	1/6		–	+
(458)	–	+	ω	+			–	–1/6		+	–
(136)		2						+	+	–	
(138)		2						+	+	–	
(168)		2						–	–	+	
(368)		2						–	–	+	
(247)		–2						+	–	+	
(257)		–2						–	+	–	
(245)		–2						+	–	+	
(457)		–2						–	+	–	

TABLE A-I (Continued)

NUMERICAL COEFFICIENTS
OF THE VARIOUS SPIN CONFIGURATIONS

S = 1											
Spin Configuration	$\Gamma_2^-\alpha$	$\Gamma_2^-\beta$	$\Gamma_3^- i$	$\Gamma_4^+\alpha, i$	$\Gamma_4^+\beta, i$	$\Gamma_4^-\alpha, i$	$\Gamma_4^-\beta, i$	$\Gamma_4^-\gamma, i$	$\Gamma_5^+\alpha, i$	$\Gamma_5^+\beta, i$	$\Gamma_5^- i$
(127)	+	+	$-\omega$		+	+	−1/2	1/6		−	+
(345)	+	+	$-\omega$		+	+	−1/2	1/6		−	+
(456)	+	+	$-\omega$		−	−	1/2	−1/6		+	−
(278)	+	+	$-\omega$		−	−	1/2	−1/6		+	−
(235)	+	+	ω^2		−	+	−1/2	1/6		−	−
(246)	+	+	1			+	1/2	−2/3		−2	
(467)	+	+	ω^2		+	−	1/2	−1/6		+	+
(248)	+	+	1			+	1/2	−2/3		−2	
(147)	+	+	ω^2		−	+	−1/2	1/6		−	−
(157)	+	+	1			−	−1/2	2/3		2	
(258)	+	+	ω^2		+	−	1/2	−1/6		+	+
(357)	+	+	1			−	−1/2	2/3		2	
(238)	−	−	$-\omega^2$		+	+	−1/2	1/6		+	−
(146)	−	−	$-\omega^2$		+	+	−1/2	1/6		+	−
(268)	−	−	−1			−	−1/2	2/3		−2	
(135)	−	−	−1			+	1/2	−2/3		2	
(356)	−	−	ω		+	−	1/2	−1/6		−	−
(346)	−	−	ω		−	+	−1/2	1/6		+	+
(128)	−	−	ω		−	+	−1/2	1/6		+	+
(468)	−	−	−1			−	−1/2	2/3		−2	
(358)	−	−	$-\omega^2$		−	−	1/2	−1/6		−	+
(178)	−	−	ω		+	−	1/2	−1/6		−	−
(167)	−	−	$-\omega^2$		−	−	1/2	−1/6		−	+
(137)	−	−	−1			+	1/2	−2/3		2	
$\lvert\Gamma_i\rvert^2$	48	80	48	16	16	32	24	16/3	16	80	32

TABLE A-I (Continued)
NUMERICAL COEFFICIENTS
OF THE VARIOUS SPIN CONFIGURATIONS

S = 0

Spin Configuration	$\Gamma_1^+\alpha$	$\Gamma_1^+\beta$	$\Gamma_1^+\gamma$	Γ_1^-	$\Gamma_3^+\alpha, i$	$\Gamma_3^+\beta, i$	$\Gamma_5^+ i$	$\Gamma_5^- i$
(1234)	+	–	3		$-2\omega^2$			
(5678)	+	–	3		$-2\omega^2$			
(1256)	+	–	3		-2ω			
(3478)	+	–	3		-2ω			
(2367)	+	–	3		-2			
(1458)	+	–	3		-2			
(2347)	–		3				–	
(1348)	–		3				–	
(1245)	–		3				+	
(1236)	–		3				+	
(3678)	–		3				+	
(4578)	–		3				+	
(1568)	–		3				–	
(2567)	–		3				–	
(1368)	+	3	3					
(2457)	+	3	3					
(1278)			8			2		
(3456)			8			2		
(1467)			8			2ω		
(2358)			8			2ω		
(1357)			8			$2\omega^2$		
(2468)			8			$2\omega^2$		

TABLE A-1 (Continued)

NUMERICAL COEFFICIENTS
OF THE VARIOUS SPIN CONFIGURATIONS

S = 0

Spin Configuration	$\Gamma_1^+\alpha$	$\Gamma_1^+\beta$	$\Gamma_1^+\gamma$	Γ_1^-	$\Gamma_3^+\alpha, i$	$\Gamma_3^+\beta, i$	$\Gamma_5^+ i$	$\Gamma_5^- i$
(2345)		–	–2		ω^2	ω^2		
(1346)		–	–2		ω^2	ω^2		
(1247)		–	–2		ω^2	ω^2		
(1238)		–	–2		ω^2	ω^2		
(1678)		–	–2		ω^2	ω^2		
(2578)		–	–2		ω^2	ω^2		
(3568)		–	–2		ω^2	ω^2		
(4567)		–	–2		ω^2	ω^2		
(1378)		–	–2		ω	ω		–
(2478)		–	–2		ω	ω		–
(3457)		–	–2		ω	ω		+
(3468)		–	–2		ω	ω		+
(1356)		–	–2		ω	ω		–
(2456)		–	–2		ω	ω		–
(1257)		–	–2		ω	ω		+
(1268)		–	–2		ω	ω		+
(1367)		–	–2		1	1	–	+
(2467)		–	–2		1	1	+	+
(2357)		–	–2		1	1	+	–
(2368)		–	–2		1	1	–	–
(2458)		–	–2		1	1	–	+
(1358)		–	–2		1	1	+	+
(1468)		–	–2		1	1	+	–
(1457)		–	–2		1	1	–	–

TABLE A-I (Continued)

NUMERICAL COEFFICIENTS
OF THE VARIOUS SPIN CONFIGURATIONS

S = 0

Spin Configuration	$\Gamma_1^+\alpha$	$\Gamma_1^+\beta$	$\Gamma_1^+\gamma$	Γ_1^-	$\Gamma_3^+\alpha, i$	$\Gamma_3^+\beta, i$	$\Gamma_5^+ i$	$\Gamma_5^- i$
(1237)		+	-2	+	$-\omega$	ω		
(2348)		+	-2	+	-1	1	+	
(1345)		+	-2	+	$-\omega$	ω		
(1246)		+	-2	+	-1	1	−	
(2678)		+	-2	+	$-\omega$	ω		
(4568)		+	-2	+	$-\omega$	ω		
(3467)		+	-2	+	$-\omega^2$	ω^2		−
(2356)		+	-2	+	$-\omega^2$	ω^2		+
(3578)		+	-2	+	-1	1	−	
(1567)		+	-2	+	-1	1	+	
(1478)		+	-2	+	$-\omega^2$	ω^2		+
(1258)		+	-2	+	$-\omega^2$	ω^2		−
(1235)		+	-2	−	-1	1	−	
(2346)		+	-2	−	$-\omega$	ω		
(1347)		+	-2	−	-1	1	+	
(1248)		+	-2	−	$-\omega$	ω		
(1267)		+	-2	−	$-\omega^2$	ω^2		−
(2568)		+	-2	−	-1	1	+	
(1456)		+	-2	−	$-\omega^2$	ω^2		+
(1578)		+	-2	−	$-\omega$	ω		
(3458)		+	-2	−	$-\omega^2$	ω^2		−
(3567)		+	-2	−	$-\omega$	ω		
(4678)		+	-2	−	-1	1	−	
(2378)		+	-2	−	$-\omega^2$	ω^2		+
$\lvert\Gamma_i\rvert^2$	16	72	720	24	72	72	24	24

APPENDIX B
MATRIX ELEMENTS

In this appendix the matrix elements of the form $(\Gamma_i|\epsilon + x\mu + y\nu|\Gamma_j)$ are given. The non-degenerate states can be obtained directly from Table I, so only the matrix elements for degenerate states are listed.

For S = 2

	$\Gamma_1^+\alpha$	$\Gamma_1^+\beta$
$\Gamma_1^+\alpha$	$-\frac{3}{2} + \frac{5}{2}x - y$	$\frac{\sqrt{7}}{2}(1-x)$
$\Gamma_1^+\beta$	$\frac{\sqrt{7}}{2}(1-x)$	$-\frac{1}{2}(1+x) + y$

	$\Gamma_3^-\alpha$, i	$\Gamma_3^-\alpha$, ii	$\Gamma_3^-\beta$, i	$\Gamma_3^-\beta$, ii
$\Gamma_3^-\alpha$, i	$(1-x)$	0	0	$-\omega(1-y)$
$\Gamma_3^-\alpha$, ii	0	$(1-x)$	$-\omega^2(1-y)$	0
$\Gamma_3^-\beta$, i	0	$-\omega(1-y)$	0	0
$\Gamma_3^-\beta$, ii	$-\omega^2(1-y)$	0	0	0

	$\Gamma_5^+\alpha$, i	$\Gamma_5^+\beta$, i
$\Gamma_5^+\alpha$, i	$\frac{1}{2}(1+x) - y$	$\frac{\sqrt{3}}{2}(1-y)$
$\Gamma_5^+\beta$, i	$\frac{\sqrt{3}}{2}(1-y)$	$-\frac{1}{2}(1+x) + y$

For S = 1

	$\Gamma_4^-\alpha, i$	$\Gamma_4^-\beta, i$	$\Gamma_4^-\gamma, i$
$\Gamma_4^-\alpha, i$	$-\frac{1}{8}(1 + 14x + y)$	$\frac{1}{8\sqrt{3}}(11 - 6x - 5y)$	$\frac{1}{4}\sqrt{\frac{5}{3}}(1 - y)$
$\Gamma_4^-\beta, i$	$\frac{1}{8\sqrt{3}}(11 - 6x - 5y)$	$\frac{1}{24}(7 - 30x - 25y)$	$\frac{5\sqrt{5}}{12}(1 - y)$
$\Gamma_4^-\gamma, i$	$\frac{1}{4}\sqrt{\frac{5}{3}}(1 - y)$	$\frac{5\sqrt{5}}{12}(1 - y)$	$\frac{1}{6}(-13 + 6x - 5y)$

	$\Gamma_4^+\alpha, i$	$\Gamma_4^+\beta, i$
$\Gamma_4^+\alpha, i$	$\frac{1}{2} - \frac{3}{2}x - y$	$-\frac{1}{2}(1 - x)$
$\Gamma_4^+\beta, i$	$-\frac{1}{2}(1 - x)$	$-\frac{3}{2}(1 + x) + y$

	$\Gamma_2^-\alpha$	$\Gamma_2^-\beta$
$\Gamma_2^-\alpha$	$-\frac{1}{4} - x - \frac{3}{4}y$	$-\frac{\sqrt{15}}{4}(1 - y)$
$\Gamma_2^-\beta$	$-\frac{\sqrt{15}}{4}(1 - y)$	$-\frac{15}{4} + 3x - \frac{5}{4}y$

	$\Gamma_5^+\alpha, i$	$\Gamma_5^+\beta, i$
$\Gamma_5^+\alpha, i$	$-\frac{3}{2} + \frac{1}{2}x - 1$	$\frac{\sqrt{5}}{2}(1 - x)$
$\Gamma_5^+\beta, i$	$\frac{\sqrt{5}}{2}(1 - x)$	$-\frac{3}{2}(1 + x) \div y$

For S = 0

	$\Gamma_1^+\alpha$	$\Gamma_1^+\beta$	$\Gamma_1^+\gamma$
$\Gamma_1^+\alpha$	$-3y$	$-\frac{3}{\sqrt{2}}(1-x)$	0
$\Gamma_1^+\beta$	$-\frac{3}{\sqrt{2}}(1-x)$	$-3+x-y$	$-\sqrt{\frac{5}{2}}(1-x)$
$\Gamma_1^+\gamma$	0	$-\sqrt{\frac{5}{2}}(1-x)$	$-2-2x+y$

	$\Gamma_3^+\alpha, i$	$\Gamma_3^+\beta, i$
$\Gamma_3^+\alpha, i$	$-2x-y$	$-(1-x)$
$\Gamma_3^+\beta, i$	$-(1-x)$	$-2-2x+y$